EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1031	(544/315,318).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2006/06/25 14:42

NPL

		Results
5.	TITLE-ABSTR-KEY(polyaniline or poly aniline) and TITLE-ABSTR-KEY(pyrimidine) *[All Sources(- All Sciences -)]*	1
4.	TITLE-ABSTR-KEY(polyaniline or poly aniline) and TITLE-ABSTR-KEY (dihydropyrimidinone) *[All Sources(- All Sciences -)]*	0
3.	TITLE-ABSTR-KEY(polyaniline or poly aniline) *[All Sources(- All Sciences -)]*	3462
2.	TITLE-ABSTR-KEY(dihydropyrimidinone) and TITLE-ABSTR-KEY(polyaniline) *[All Sources(- All Sciences -)]*	0
1.	TITLE-ABSTR-KEY(dihydropyrimidinone) *[All Sources(- All Sciences -)]*	73

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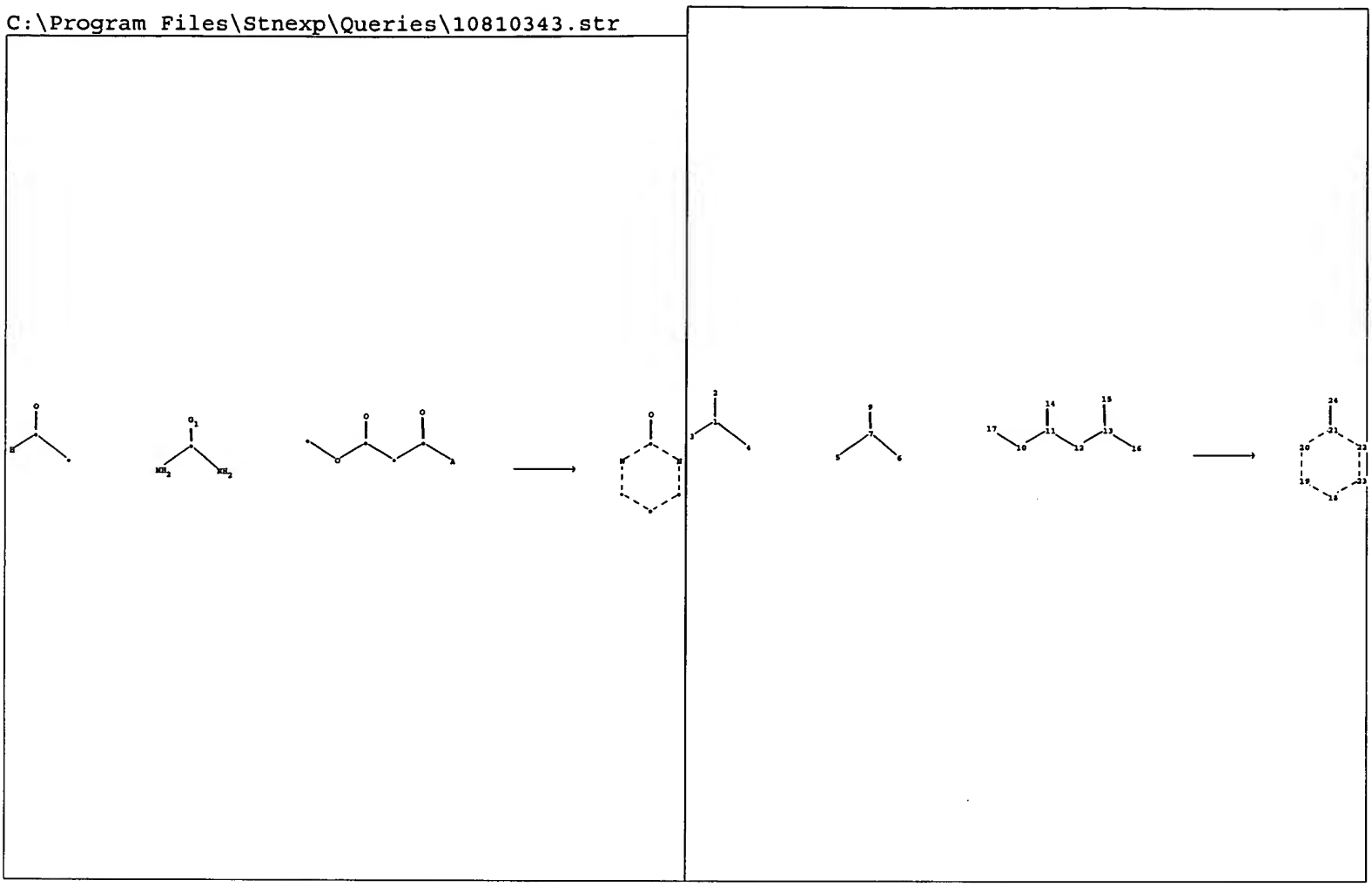
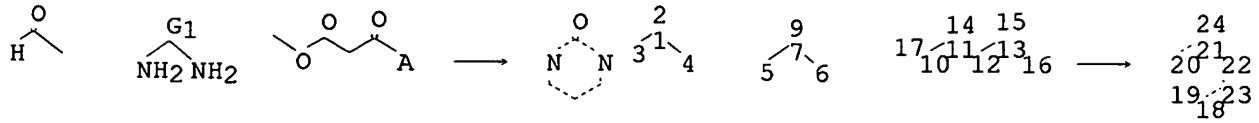


chain nodes :
1 2 3 5 6 7 9 10 11 12 13 14 15 24
ring nodes :
18 19 20 21 22 23
ring/chain nodes :
4 16 17
chain bonds :
1-2 1-3 1-4 5-7 6-7 7-9 10-11 10-17 11-12 11-14 12-13 13-15 13-16 21-24
ring bonds :
18-19 18-23 19-20 20-21 21-22 22-23
exact/norm bonds :
1-2 5-7 6-7 7-9 10-11 10-17 11-14 13-15 13-16 18-19 18-23 19-20 20-21 21-22
21-24 22-23
exact bonds :
1-3 1-4 11-12 12-13
isolated ring systems :
containing 18 :

G1:O,S

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:CLASS
fragments assigned product role:
containing 18
fragments assigned reactant/reagent role:
containing 1
containing 5
containing 10

=>
Uploading C:\Program Files\Stnexp\Queries\10810343.str



chain nodes :
1 2 3 5 6 7 9 10 11 12 13 14 15 24
ring nodes :
18 19 20 21 22 23
ring/chain nodes :
4 16 17
chain bonds :
1-2 1-3 1-4 5-7 6-7 7-9 10-11 10-17 11-12 11-14 12-13 13-15 13-16
21-24
ring bonds :
18-19 18-23 19-20 20-21 21-22 22-23
exact/norm bonds :
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21-22 21-24 22-23
exact bonds :
1-3 1-4 11-12 12-13
isolated ring systems :
containing 18 :

G1:O,S

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS
fragments assigned product role:
containing 18
fragments assigned reactant/reagent role:
containing 1
containing 5
containing 10

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

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=> s l1 sss sam
SAMPLE SEARCH INITIATED 13:24:00 FILE 'CASREACT'
SCREENING COMPLETE -     282 REACTIONS TO VERIFY FROM       23 DOCUMENTS

100.0% DONE     282 VERIFIED      95 HIT RXNS                      6 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:      4633 TO     6647
PROJECTED ANSWERS:               6 TO      266

L2            6 SEA SSS SAM L1 (    95 REACTIONS)

=> => s l1 sss ful
FULL SEARCH INITIATED 13:26:41 FILE 'CASREACT'
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100.0% DONE    4674 VERIFIED    2079 HIT RXNS                    186 DOCS
SEARCH TIME: 00.00.01

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=> s polyanilin? or anilin?
           67 POLYANILIN?
        17462 ANILIN?
L4      17505 POLYANILIN? OR ANILIN?

=> s l3 and l4
L5           5 L3 AND L4

=> d l5 1-5 bib,ab,crdref
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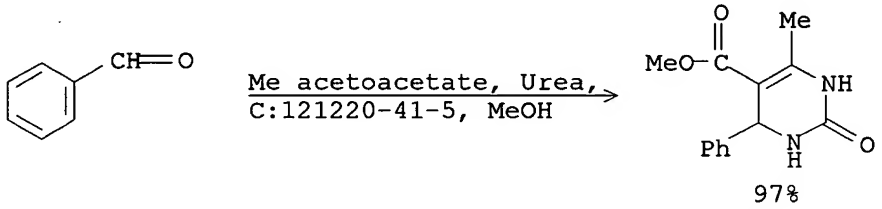
L5 ANSWER 1 OF 5 CASREACT COPYRIGHT 2006 ACS on STN
AN 143:347196 CASREACT
TI Preparation of substituted dihydropyrimidinones from aldehydes, ketoesters, and urea/thiourea using **polyaniline** salts as catalysts.
IN Srinivasan, Palaniappan; Rao, Vaidya J.; Banda, Gangadasu
PA Council of Scientific and Industrial Research, India
SO U.S. Pat. Appl. Publ., 6 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2005215790	A1	20050929	US 2004-810343	20040326
PRAI US 2004-810343		20040326		

Appl pg Pub.

AB A process for the preparation of substituted dihydropyrimidinones and dihydropyrimidinethiones comprises reaction of an aldehyde, a β-keto ester, and urea/thiourea in the presence of a **polyaniline** salt catalyst. Thus, PhCHO, Me acetoacetate, urea, and **polyaniline** tosylate were refluxed 120 min. in MeOH to give 97% product.

RX(1) OF 17



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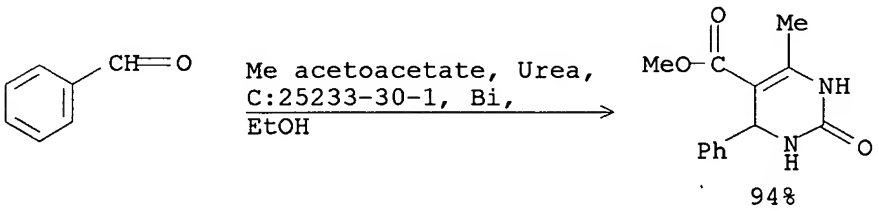
REF: U.S. Pat. Appl. Publ., 2005215790, 29 Sep 2005
NOTE: optimization study
CON: 2 hours, 64 deg C

RX(2) OF 17



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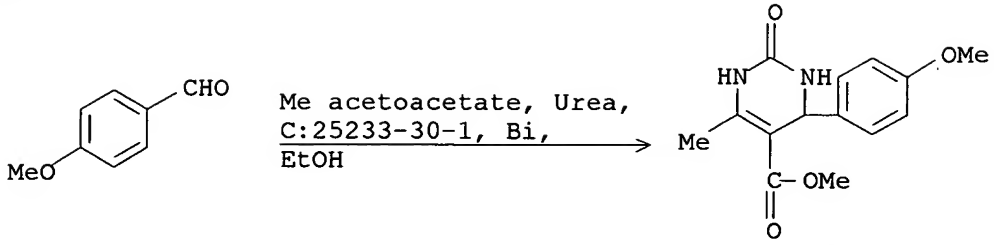
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 2 hours, reflux

RX(3) OF 17



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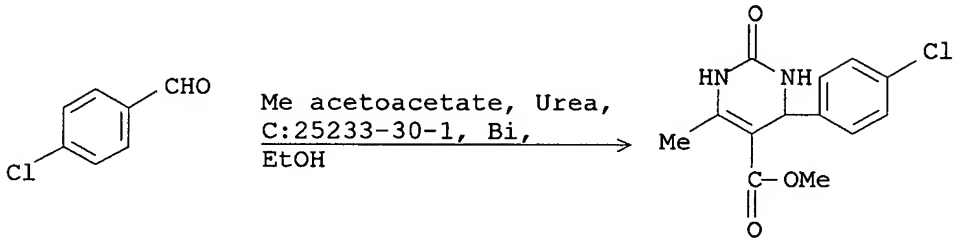
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 2 hours, reflux

RX(4) OF 17



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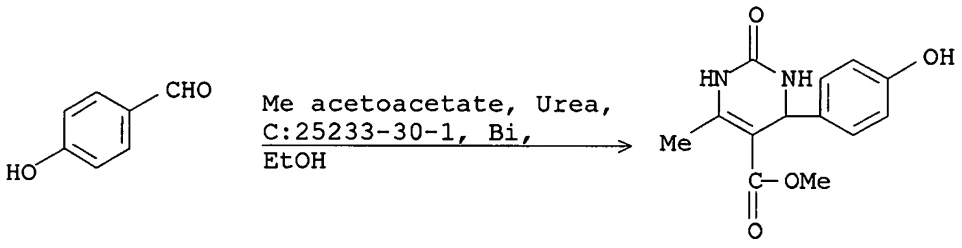
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 5 hours, reflux

RX(5) OF 17



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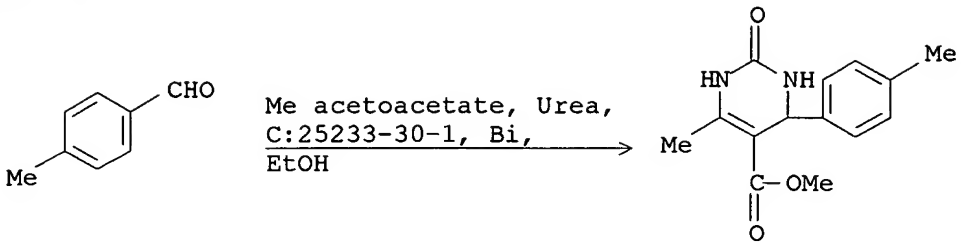
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 5 hours, reflux

RX(6) OF 17



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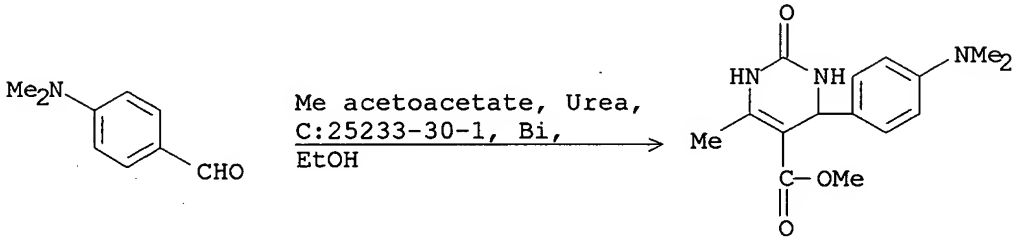
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 4 hours, reflux

RX(7) OF 17



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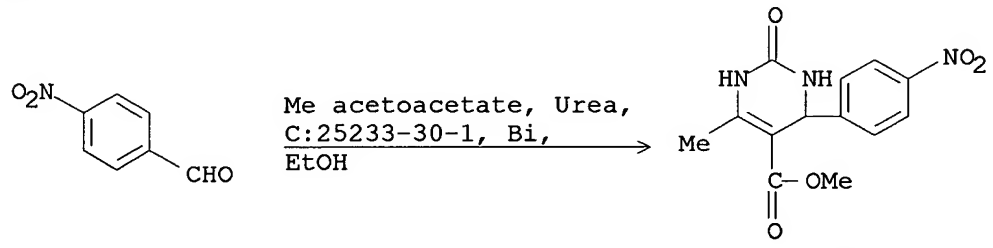
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 6 hours, reflux

RX(8) OF 17



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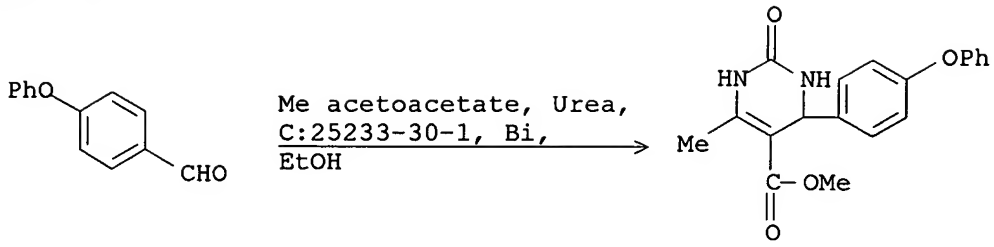
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 6 hours, reflux

RX(9) OF 17



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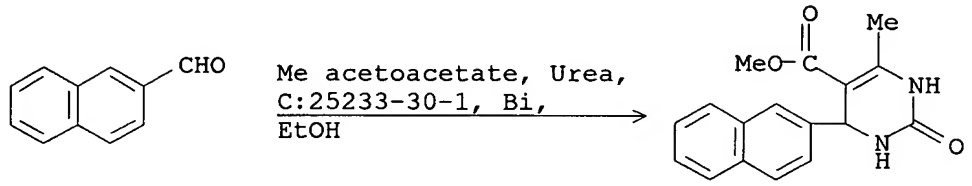
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 4 hours, reflux

RX(10) OF 17



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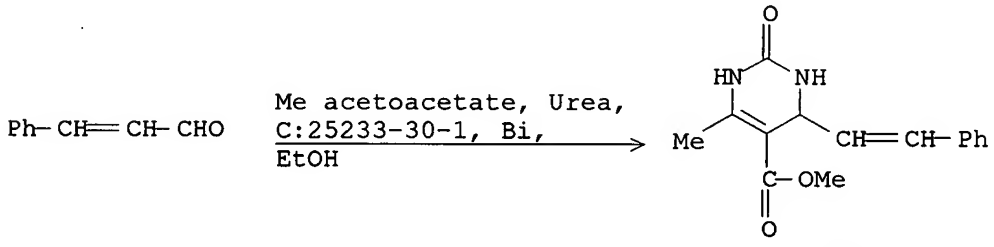
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 5 hours, reflux

RX(11) OF 17



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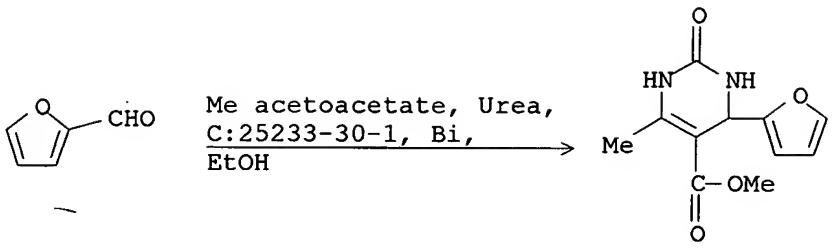
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 4 hours, reflux

RX(12) OF 17



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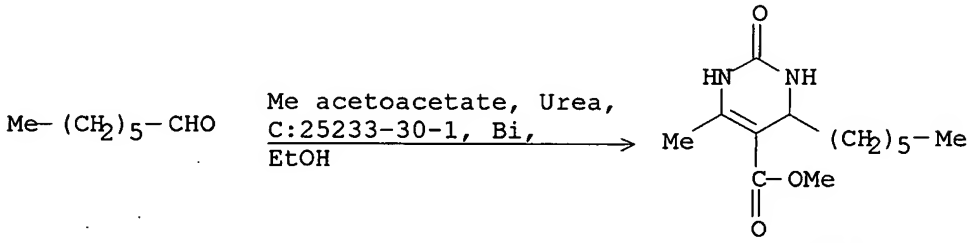
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 4 hours, reflux

RX(13) OF 17



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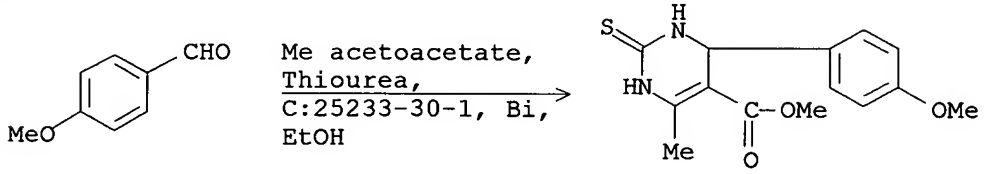
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 4 hours, reflux

RX(14) OF 17



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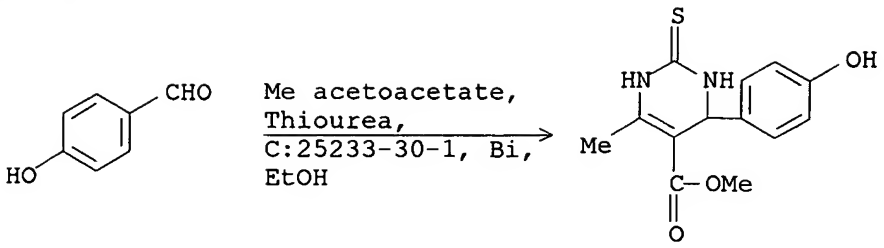
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 4 hours, reflux

RX(15) OF 17



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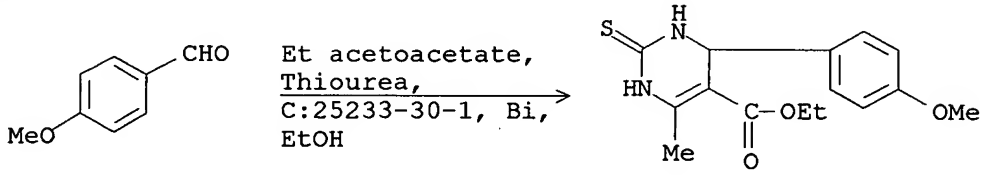
REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 6 hours, reflux

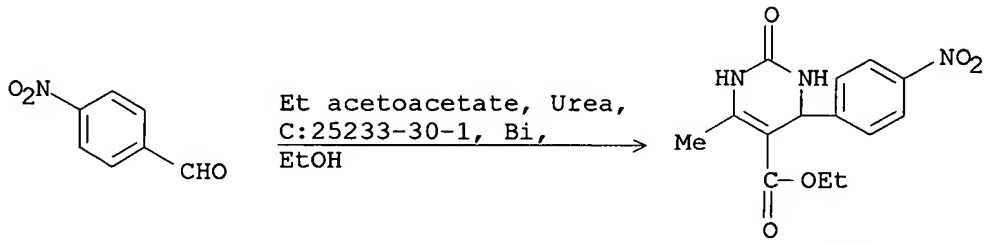
RX(16) OF 17



84%

REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 4 hours, reflux

RX(17) OF 17



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REF: U.S. Pat. Appl. Publ., 6 pp.; 2005
NOTE: catalyst is polyaniline-bismuth trichloride
CON: 6 hours, reflux

L5 ANSWER 2 OF 5 CASREACT COPYRIGHT 2006 ACS on STN
AN 143:133385 CASREACT
TI A preparation of dihydropyrimidinone derivatives from β-ketoester and (thio)urea in the presence of **polyaniline** salts
IN Palaniappan, Srinivasan; Rao, Vaidya Jayathirtha; Banda, Gangadasu
PA Council of Scientific & Industrial Research, India
SO PCT Int. Appl., 12 pp.
CODEN: PIXXD2
DT Patent
LA English

Same Inv. Appl PCT.

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005063719	A1	20050714	WO 2003-IN455	20031231
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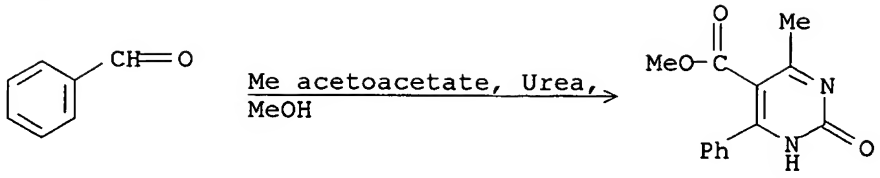
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2003300711	A1	20050721	AU 2003-300711	20031231

PRAI WO 2003-IN455 20031231

AB The invention relates to a preparation of dihydropyrimidinone derivs. from β-ketoester and (thio)urea in the presence of **polyaniline** salts as reusable catalysts. For instance, substituted dihydropyrimidinones were prepared via heterocyclization of urea, benzaldehyde, and Me acetoacetate in the presence of the prepared **polyaniline**-p-toluene sulfonate salt powder with a yield of 97% (reaction time: 120 min). A significant advantage of the invention is that the catalyst can be recycled to reaction mixture without significant loss in activity.

RX(1) OF 20



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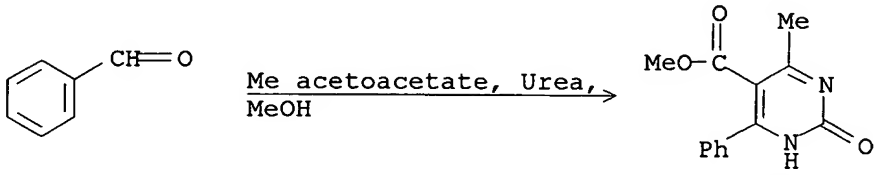
REF: PCT Int. Appl., 2005063719, 14 Jul 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 120 minutes, reflux

RX(2) OF 20



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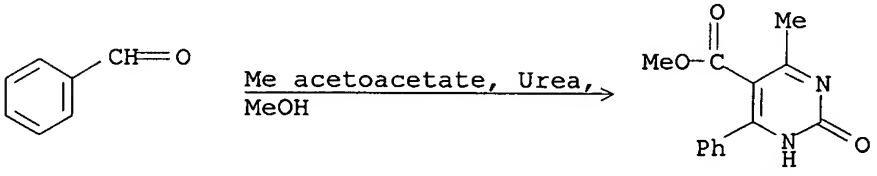
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 2 hours, 64 deg C

RX(3) OF 20



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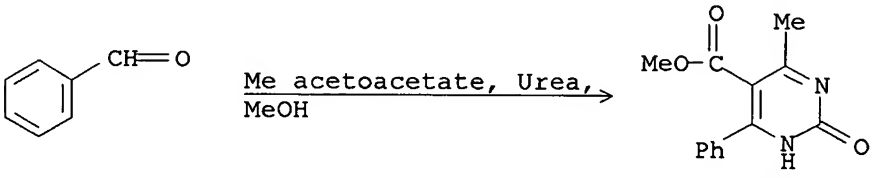
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 2 hours, reflux

RX(4) OF 20



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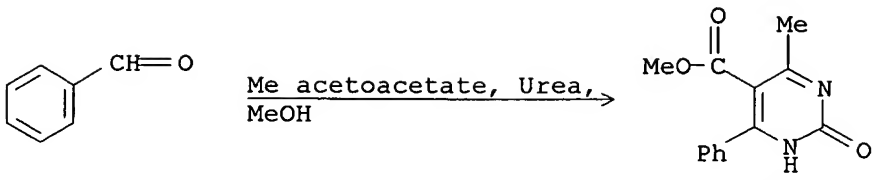
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 2 hours, reflux

RX(5) OF 20



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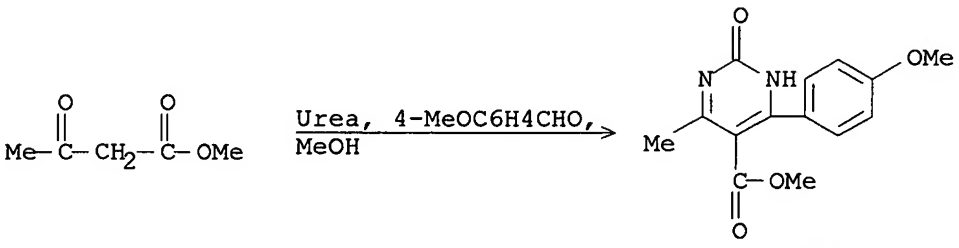
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 2 hours, reflux

RX(6) OF 20



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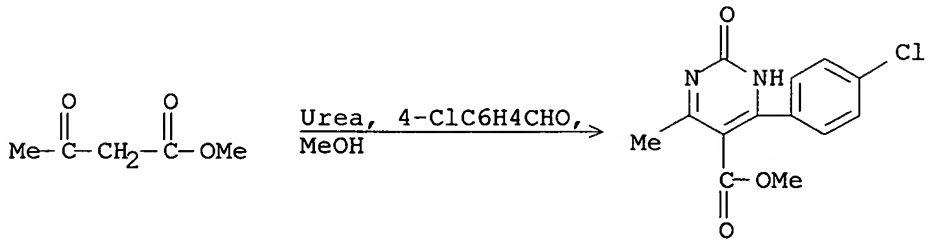
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 2 hours, reflux

RX(7) OF 20



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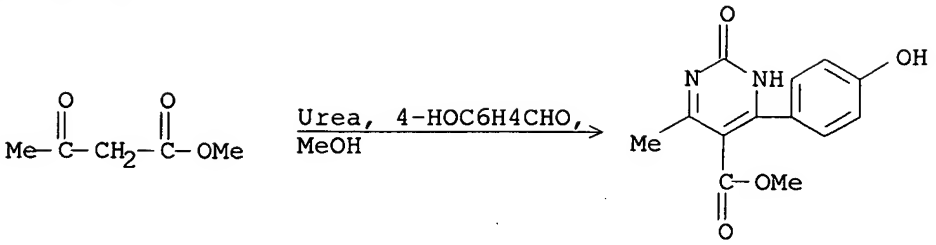
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 5 hours, reflux

RX(8) OF 20



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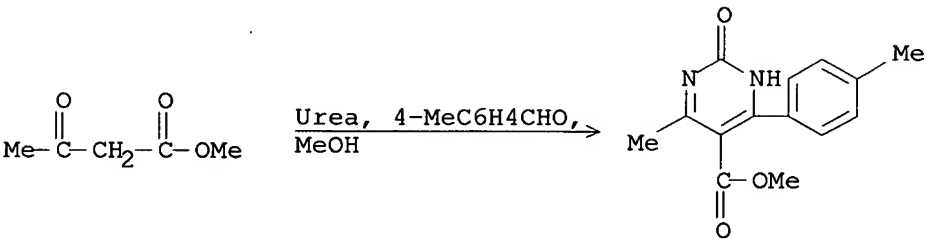
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 5 hours, reflux

RX(9) OF 20



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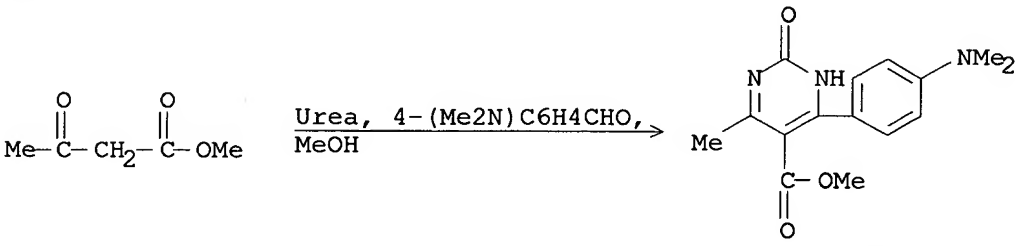
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 4 hours, reflux

RX(10) OF 20



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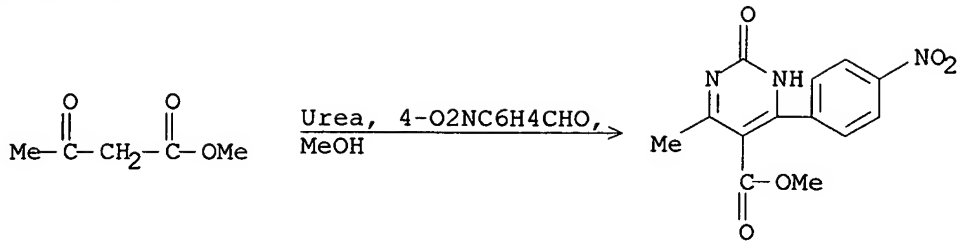
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 6 hours, reflux

RX(11) OF 20



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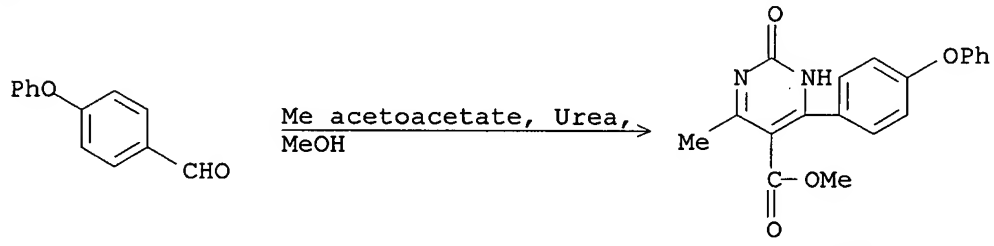
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 6 hours, reflux

RX(12) OF 20



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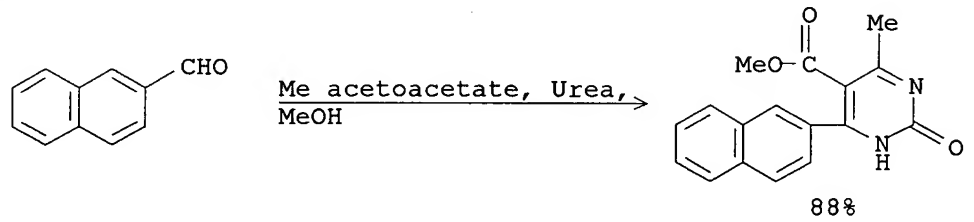
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 4 hours, reflux

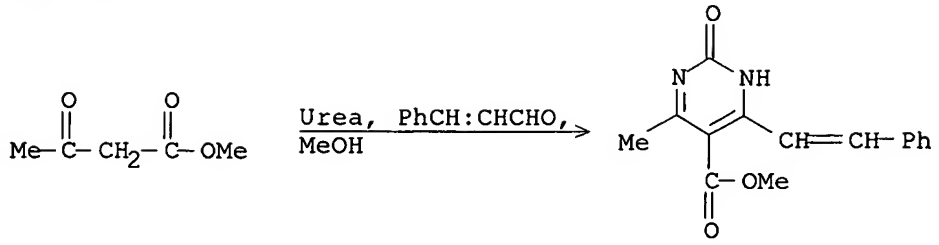
RX(13) OF 20



88%

REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 5 hours, reflux

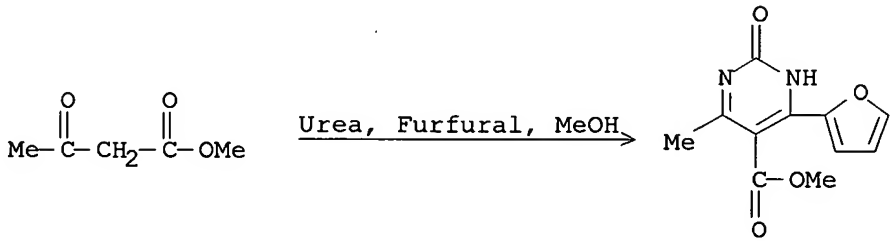
RX(14) OF 20



98%

REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 4 hours, reflux

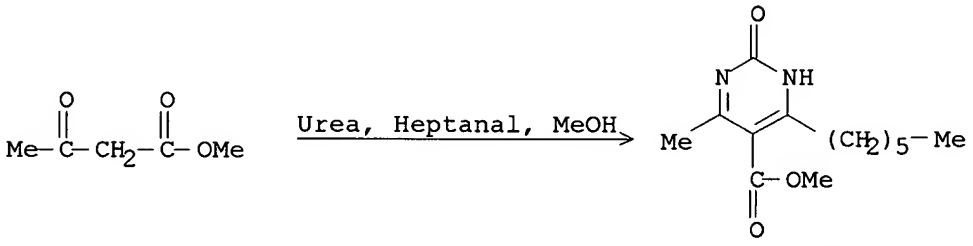
RX(15) OF 20



85%

REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 4 hours, reflux

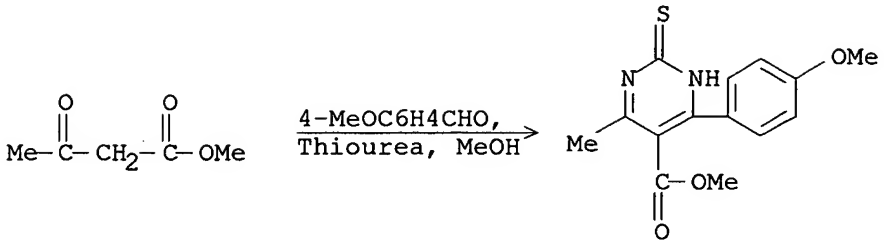
RX(16) OF 20



86%

REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 4 hours, reflux

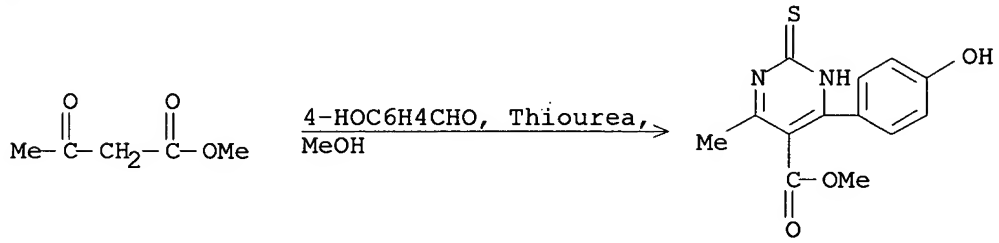
RX(17) OF 20



85%

REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 4 hours, reflux

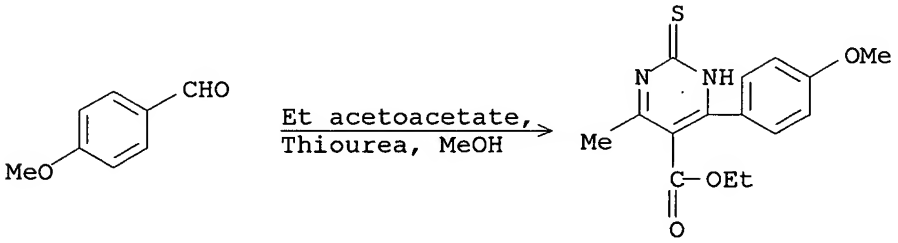
RX(18) OF 20



82%

REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 6 hours, reflux

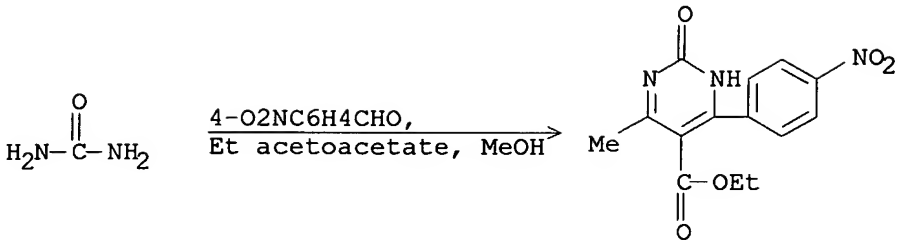
RX(19) OF 20



84%

REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 4 hours, reflux

RX(20) OF 20



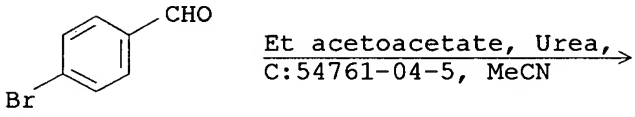
82%

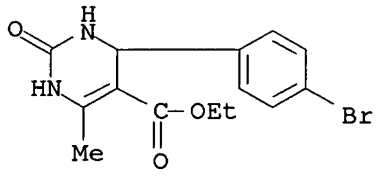
REF: PCT Int. Appl., 12 pp.; 2005
NOTE: polyaniline-bismuth trichloride powder used as catalyst, green chem.-recyclable catalyst
CON: 6 hours, reflux

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 5 CASREACT COPYRIGHT 2006 ACS on STN
AN 143:26558 CASREACT
TI Microwave-Enhanced and Metal-Catalyzed Functionalizations of the 4-Aryl-Dihydropyrimidone Template
AU Wannberg, Johan; Dallinger, Doris; Kappe, C. Oliver; Larhed, Mats
CS Department of Medicinal Chemistry Organic, Pharmaceutical Chemistry, BMC, Uppsala University, Uppsala, Swed.
SO Journal of Combinatorial Chemistry (2005), 7(4), 574-583
CODEN: JCCHFF; ISSN: 1520-4766
PB American Chemical Society
DT Journal
LA English
AB Progress in organometallic catalysis and recent advancements in the development of carbonylative reaction protocols without direct use of carbon monoxide have been utilized for efficient functionalizations of 4-aryldihydropyrimidone structures. The use of modern microwave technol. enabled both high reaction rates and convenient handling. Examples of palladium-catalyzed cross-couplings, Heck reactions, amino- and alkoxycarbonylations, and direct N-amidations of 4-(bromophenyl)-dihydropyrimidones I (R1 = R2 = H; X = Br) with formation of I (R1 = R2 = H; X = MeO2C, MeCONH, BuNHCO, MeO2CCH:CH, Ph, PhCONH, PhCONHNHCO, etc.) were performed. Further, the first N3-arylations of the dihydropyrimidone ring system in I (R1 = H, Me; R2 = X = H) to give I (R1 = H, Me; R2 = Ph, 3-MeOC6H4, 4-O2NC6H4, etc.; X = H) were successfully completed using the copper-catalyzed Goldberg reaction. Altogether, these protocols provide new tools for rapid generation of novel and diverse dihydropyrimidone derivs.

RX(1) OF 60

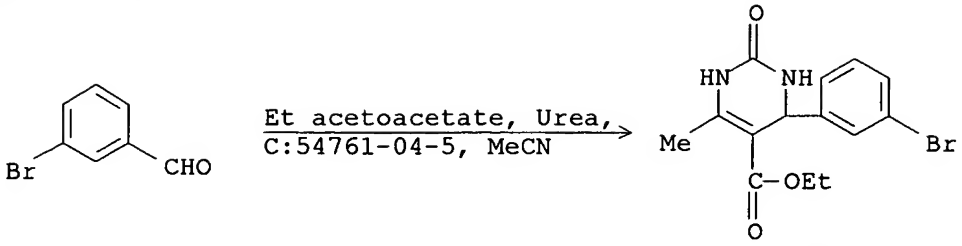




77%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: microwave irradn.
CON: 15 minutes, 120 deg C

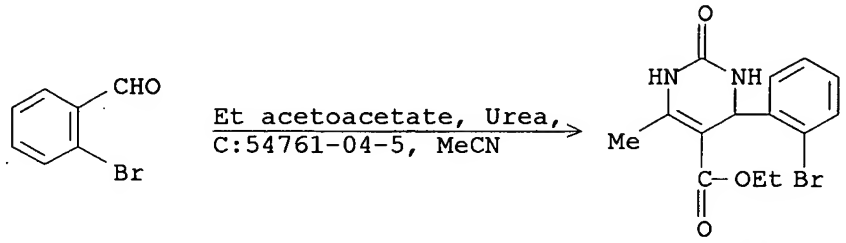
RX(2) OF 60



85%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: microwave irradn.
CON: 15 minutes, 120 deg C

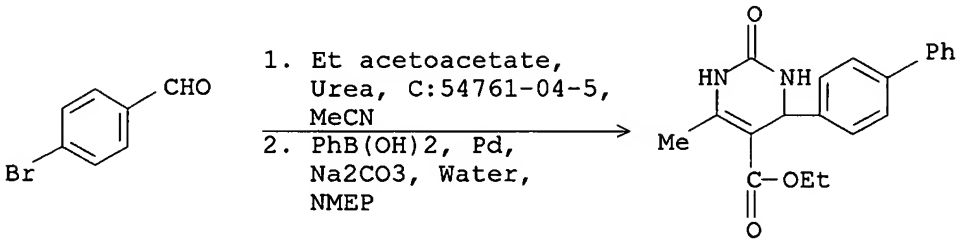
RX(3) OF 60



73%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: microwave irradn.
CON: 15 minutes, 120 deg C

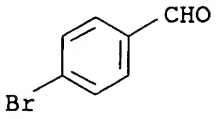
RX(37) OF 60 - 2 STEPS



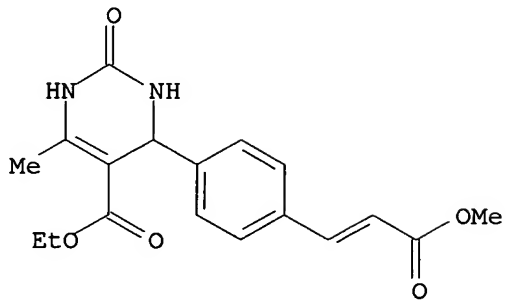
70%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 20 minutes, 120 deg C

RX(38) OF 60 - 2 STEPS



1. Et acetoacetate, Urea, C:54761-04-5, MeCN
2.1. Pd(OAc)2, Tri-o-tolylphosphine, EtN(Pr-i)2, MeCN
2.2. Me acrylate

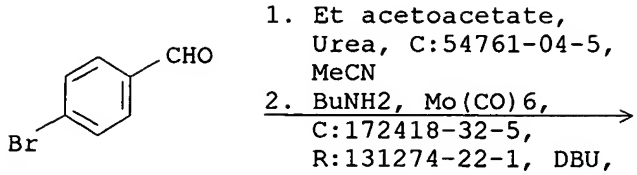


65%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005

NOTE: 1) microwave irradn., 2) microwave irradn. second stage
CON: STEP(1) 15 minutes, 120 deg C
STEP(2.1) 45 minutes, 60 deg C
STEP(2.2) 30 minutes, 180 deg C

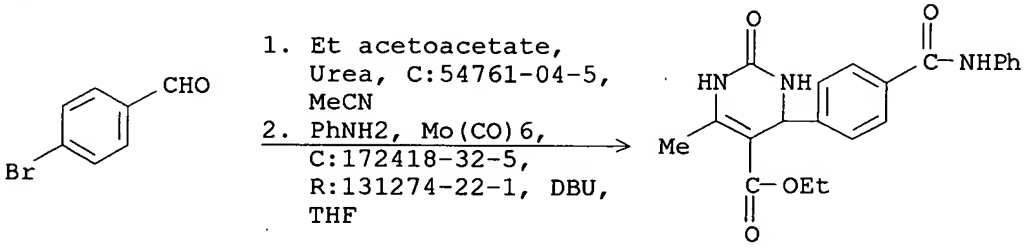
RX(39) OF 60 - 2 STEPS



87%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 130 deg C

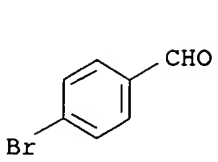
RX(40) OF 60 - 2 STEPS



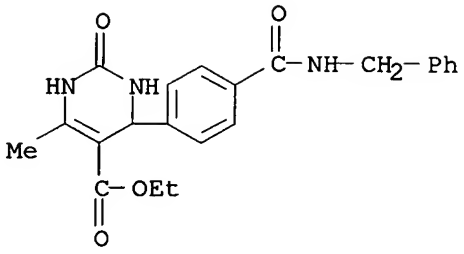
83%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 130 deg C

RX(41) OF 60 - 2 STEPS



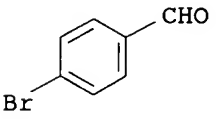
1. Et acetoacetate, Urea, C:54761-04-5, MeCN
2. PhCH2NH2, Mo(CO)6, C:172418-32-5, R:131274-22-1, DBU, THF



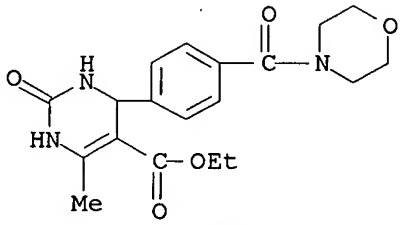
78%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 130 deg C

RX(42) OF 60 - 2 STEPS



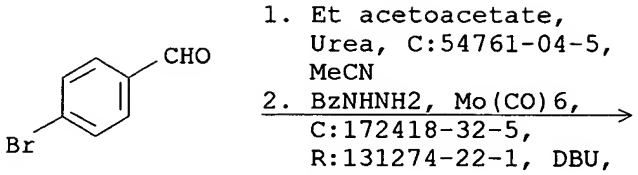
1. Et acetoacetate, Urea, C:54761-04-5, MeCN
2. Morpholine, Mo(CO)6, C:172418-32-5, R:131274-22-1, DBU, THF



56%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 140 deg C

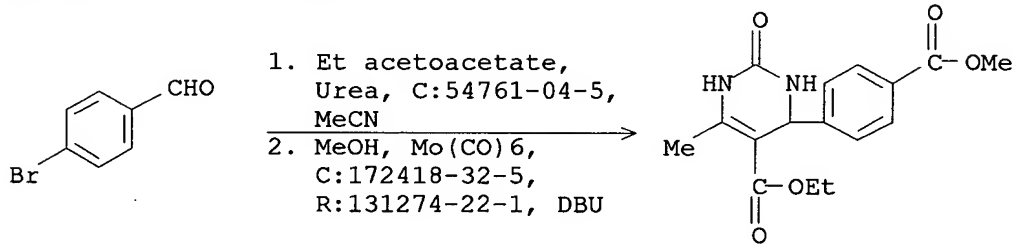
RX(43) OF 60 - 2 STEPS



35%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 5 minutes, 130 deg C

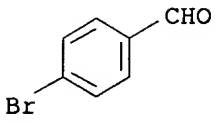
RX(44) OF 60 - 2 STEPS



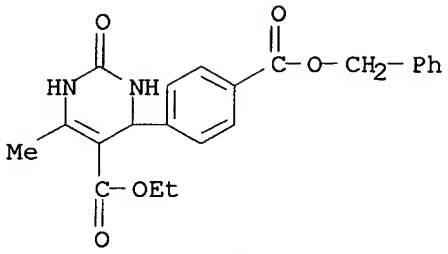
77%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 110 deg C

RX(45) OF 60 - 2 STEPS



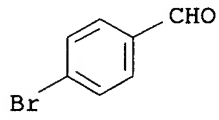
1. Et acetoacetate, Urea, C:54761-04-5, MeCN
2. PhCH2OH, Mo(CO)6, C:172418-32-5, R:131274-22-1, DBU, THF



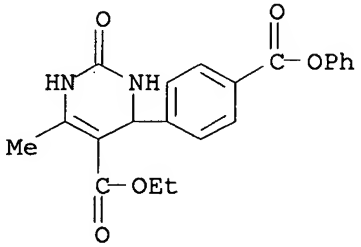
45%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 140 deg C

RX(46) OF 60 - 2 STEPS



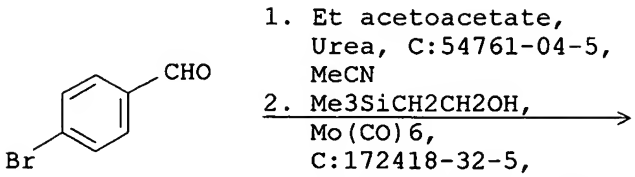
1. Et acetoacetate, Urea, C:54761-04-5, MeCN
2. PhOH, Mo(CO)6, C:172418-32-5, R:131274-22-1, DBU, THF

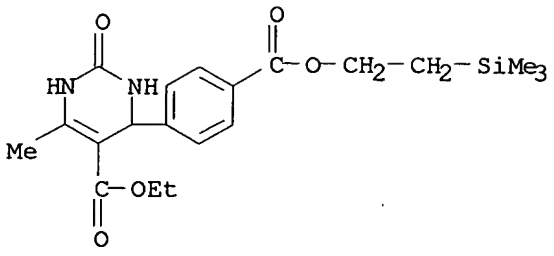


42%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 140 deg C

RX(47) OF 60 - 2 STEPS

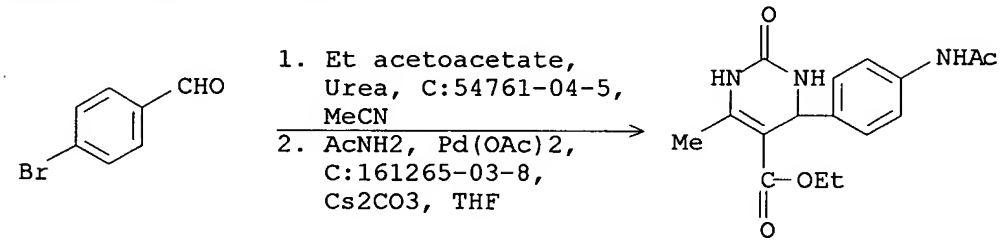




52%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 140 deg C

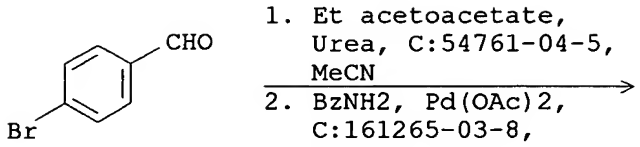
RX(48) OF 60 - 2 STEPS

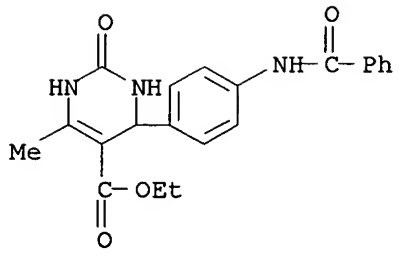


85%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 140 deg C

RX(49) OF 60 - 2 STEPS

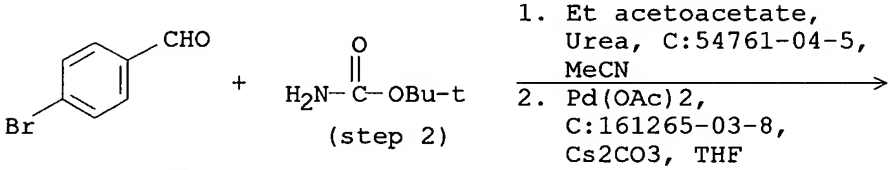


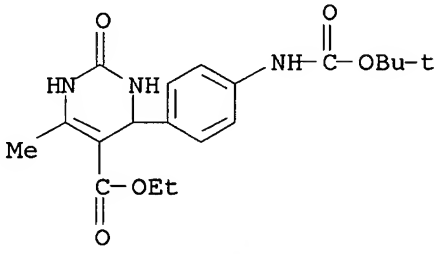


72%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 120 deg C

RX(50) OF 60 - 2 STEPS

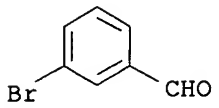




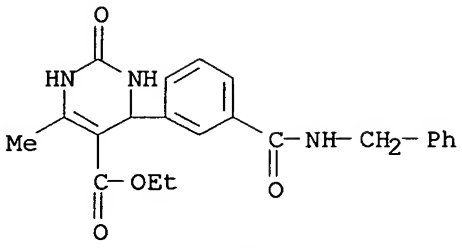
62%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 150 deg C

RX(51) OF 60 - 2 STEPS



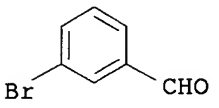
1. Et acetoacetate, Urea, C:54761-04-5, MeCN
2. PhCH2NH2, Mo(CO)6, C:172418-32-5, R:131274-22-1, DBU, THF



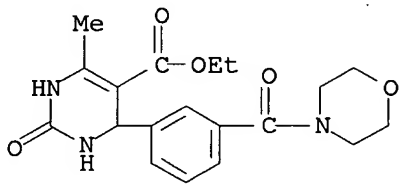
65%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 130 deg C

RX(52) OF 60 - 2 STEPS



1. Et acetoacetate, Urea, C:54761-04-5, MeCN
2. Morpholine, Mo(CO)6, C:172418-32-5, R:131274-22-1, DBU, THF



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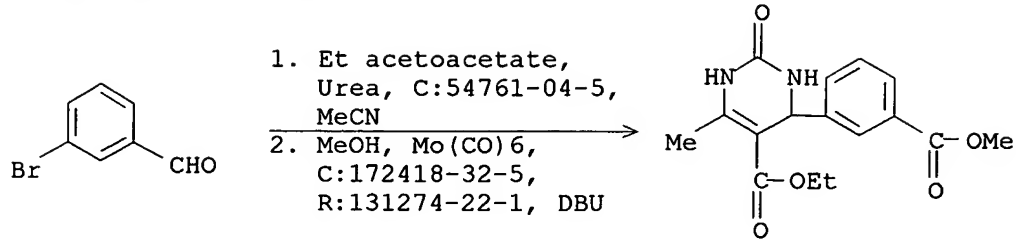
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 140 deg C

RX(53) OF 60 - 2 STEPS



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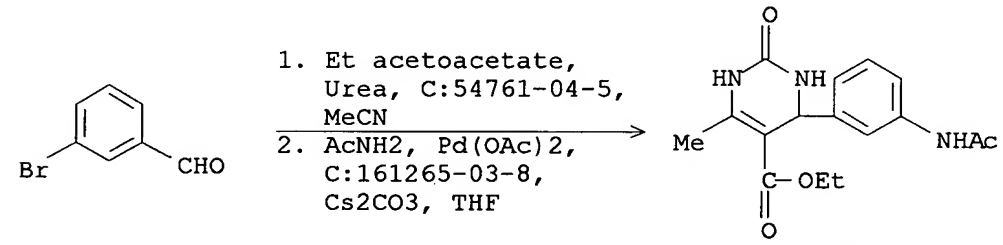
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 110 deg C

RX(54) OF 60 - 2 STEPS



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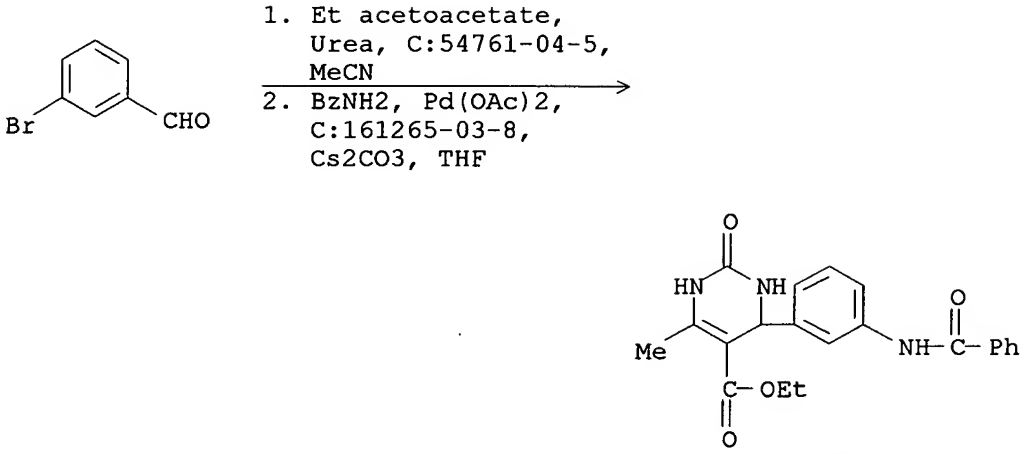
REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 140 deg C

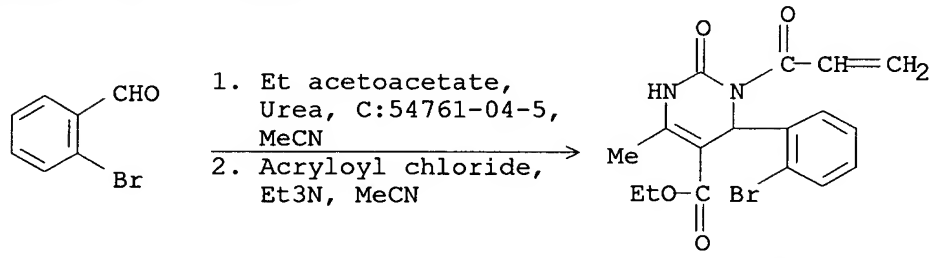
RX(55) OF 60 - 2 STEPS



88%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 120 deg C

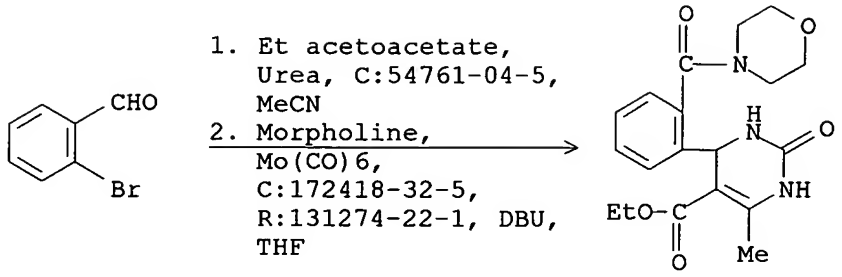
RX(56) OF 60 - 2 STEPS



62%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn., regioselective
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 20 minutes, 180 deg C

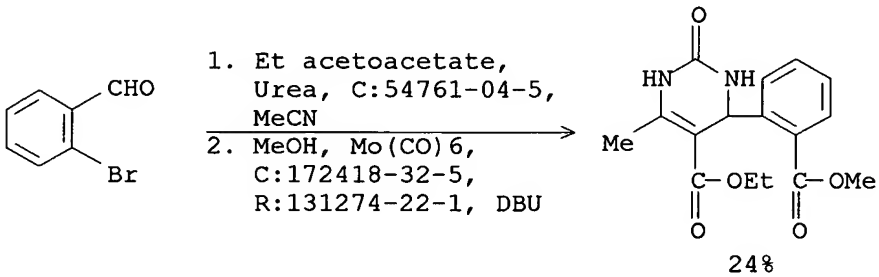
RX(57) OF 60 - 2 STEPS



21%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 140 deg C

RX(58) OF 60 - 2 STEPS



24%

REF: Journal of Combinatorial Chemistry, 7(4), 574-583; 2005
NOTE: 1) microwave irradn., 2) microwave irradn.
CON: STEP(1) 15 minutes, 120 deg C
STEP(2) 15 minutes, 120 deg C

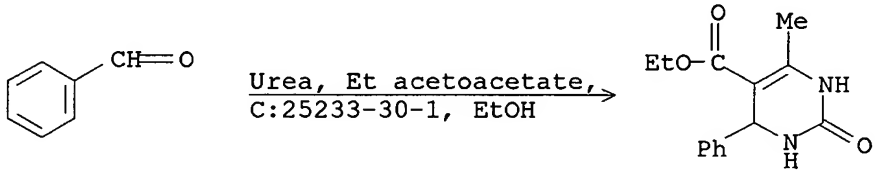
RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 5 CASREACT COPYRIGHT 2006 ACS on STN
AN 141:207164 CASREACT
TI One-pot synthesis of dihydropyrimidinones using **polyaniline** -bismoclite complex. A facile and reusable catalyst for the Biginelli reaction
AU Gangadasu, Banda; Palaniappan, Srinivasan; Rao, Vaidya Jayathirtha
CS Organic Chemistry Division II, Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SO Synlett (2004), (7), 1285-1287
CODEN: SYNLES; ISSN: 0936-5214
PB Georg Thieme Verlag
DT Journal
LA English

June, 2004 Not prior

AB **Polyaniline**-bismoclite complex was used as an efficient catalyst for the three-component condensation reaction of an aldehyde, β-ketoester, and urea in ethanol to afford the dihydropyrimidinones in excellent yields. Furthermore, after completion of reaction the catalyst could be easily recovered and reused without affecting its activity.

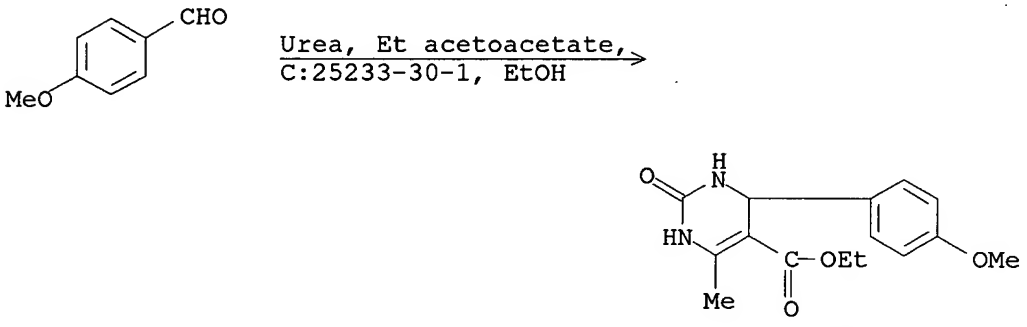
RX(1) OF 14



94%

REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 2 hours

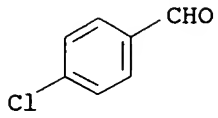
RX(2) OF 14



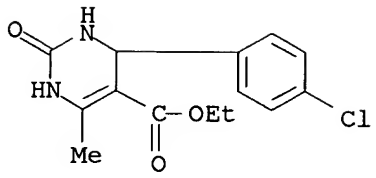
98%

REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 2 hours

RX(3) OF 14



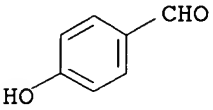
Urea, Et acetoacetate,
C:25233-30-1, EtOH



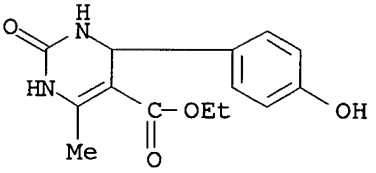
88%

REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 5 hours

RX(4) OF 14



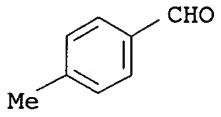
Urea, Et acetoacetate,
C:25233-30-1, EtOH



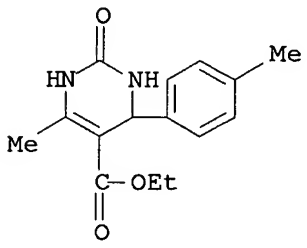
92%

REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 5 hours

RX(5) OF 14



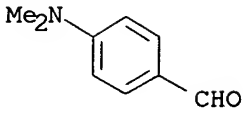
Urea, Et acetoacetate,
C:25233-30-1, EtOH



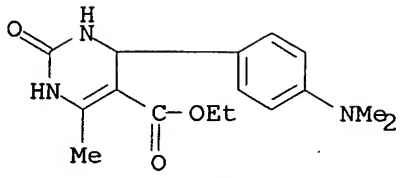
96%

REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 4 hours

RX(6) OF 14



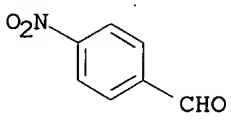
Urea, Et acetoacetate,
C:25233-30-1, EtOH



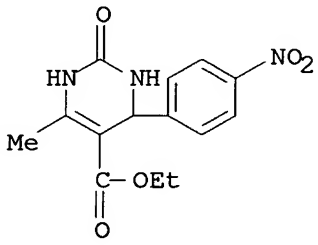
93%

REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 6 hours

RX(7) OF 14



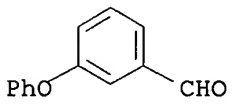
Urea, Et acetoacetate,
C:25233-30-1, EtOH



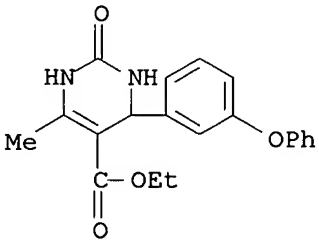
93%

REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 6 hours

RX(8) OF 14



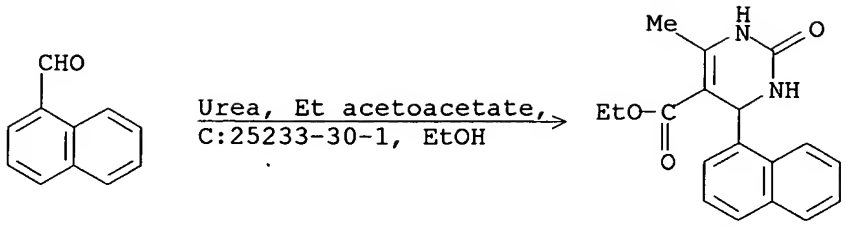
Urea, Et acetoacetate,
C:25233-30-1, EtOH



96%

REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 4 hours

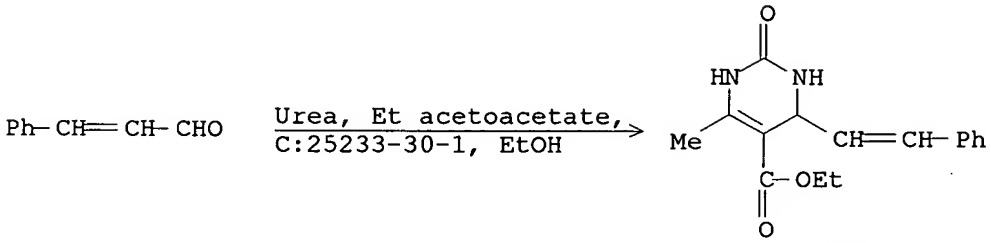
RX(9) OF 14



88%

REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 5 hours

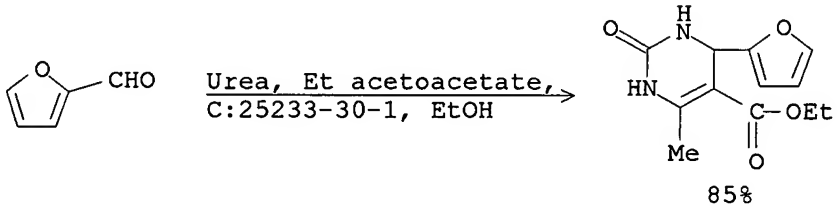
RX(10) OF 14



98%

REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 4 hours

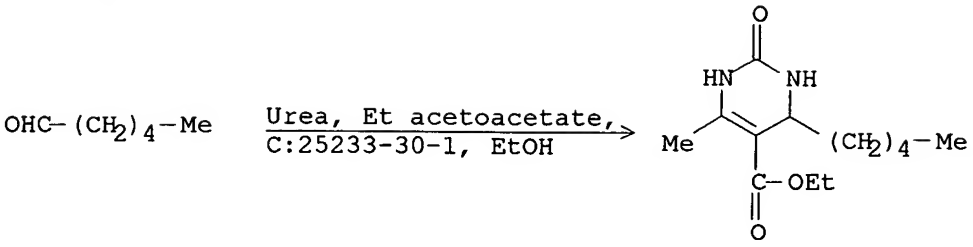
RX(11) OF 14



85%

REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 4 hours

RX(12) OF 14



86%

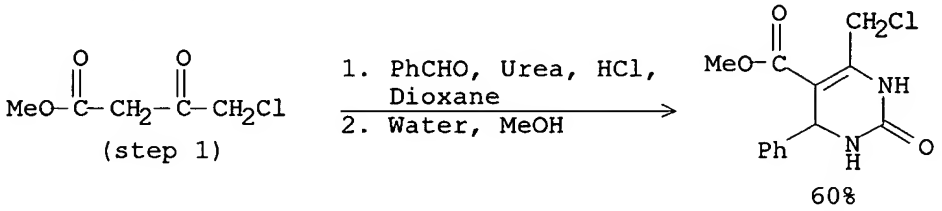
REF: Synlett, (7), 1285-1287; 2004
NOTE: heated, Biginelli reaction
CON: 4 hours

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 5 CASREACT COPYRIGHT 2006 ACS on STN
AN 137:232612 CASREACT
TI Traceless Solid-Phase Synthesis of Bicyclic Dihydropyrimidones Using Multidirectional Cyclization Cleavage
AU Perez, Rolando; Beryozkina, Tetyana; Zbruyev, Oleksandr I.; Haas, Wilhelm; Kappe, C. Oliver
CS Institute of Chemistry, Karl-Franzens-University Graz, Graz, A-8010, Austria
SO Journal of Combinatorial Chemistry (2002), 4(5), 501-510
CODEN: JCCHFF; ISSN: 1520-4766
PB American Chemical Society
DT Journal
LA English
AB Furopyrimidinediones I [R = Ph, 4-MeC6H4, 2-ClC6H4, 3-O2NC6H4, 4-FC6H4, 2,3-Cl2C6H3, 3,4-F2C6H3, 2-naphthyl, 2-F3CC6H4, 4-BrC6H4, 3,4-(MeO)2C6H3, 2-thienyl], pyrrolopyrimidinediones II [R = Ph, 4-MeC6H4, 2-ClC6H4, 3-O2NC6H4, 4-FC6H4, 3,4-F2C6H3, 2-naphthyl, 4-BrC6H4, 3,4-(MeO)2C6H3, 2-thienyl; R1 = EtCH2, Me2CHCH2CH2, HOCH2CH2, H2C:CHCH2, c-C6H11, Ph, PhCH2, 3-MeC6H4CH2, 2-ClC6H4CH2, 2-MeOC6H4CH2CH2, 4-FC6H4CH2CH2], and pyrimidopyridazinediones III [R = Ph, 4-MeC6H4, 2-ClC6H4, 4-FC6H4, 3,4-F2C6H3, 4-BrC6H4, 3,4-(MeO)2C6H3, 2-thienyl; R2 = H, Me, Ph] were prepared by solid- and solution-phase synthetic procedures using the Biginelli condensation reaction as the key steps. Condensation of aromatic aldehydes, and urea neat in the presence of HCl yielded the intermediate chloromethyl oxodihydropyrimidinecarboxylates IV [R = Ph, 4-MeC6H4, 2-ClC6H4, 3-O2NC6H4, 4-FC6H4, 2,3-Cl2C6H3, 3,4-F2C6H3, 2-naphthyl] in 27-72% yields; heating IV neat at 210° yielded I [R = Ph, 4-MeC6H4, 2-ClC6H4, 3-O2NC6H4, 4-FC6H4, 2,3-Cl2C6H3, 3,4-F2C6H3, 2-naphthyl] in 58-72% yields. Treatment of IV [R = Ph, 4-MeC6H4, 2-ClC6H4, 3-O2NC6H4, 4-FC6H4, 2,3-Cl2C6H3, 3,4-F2C6H3, 2-naphthyl] with amines in MeOH provided II [R = Ph, 4-MeC6H4, 2-ClC6H4, 3-O2NC6H4, 4-FC6H4, 2,3-Cl2C6H3, 3,4-F2C6H3, 2-naphthyl; R1 = EtCH2, HOCH2CH2, H2C:CHCH2, c-C6H11, PhCH2, 3-MeC6H4CH2, 2-ClC6H4CH2, 2-MeOC6H4CH2CH2, 4-FC6H4CH2CH2] in 33-74% yields; treatment of IV with hydrazines in dioxane or EtOH yielded III [R = Ph, 4-MeC6H4, 2-ClC6H4, 4-FC6H4, 3,4-F2C6H3; R2 = H, Me, Ph] in 26-82% yields. The solid-phase sequence involves the initial high-speed, microwave-promoted acetoacetylation of hydroxymethylpolystyrene resin with Me 4-chloroacetoacetate to give a resin-bound chloroacetoacetate ester; three-component Biginelli-type condensations with urea and aromatic aldehydes yielded resin-bound chloromethyl oxodihydropyrimidinecarboxylates. Microwave flash heating of resin-bound chloromethyl oxodihydropyrimidinecarboxylates for 10 min at 150° yielded I [R = Ph, 4-MeC6H4, 2-ClC6H4, 3-O2NC6H4, 4-FC6H4, 2,3-Cl2C6H3, 3,4-F2C6H3, 2-naphthyl, 2-F3CC6H4, 4-BrC6H4, 3,4-(MeO)2C6H3, 2-thienyl] in 14-77% yields. Addition of amines to the resin-bound chloromethyl oxodihydropyrimidinecarboxylate intermediates at either ambient temperature or at 50° gave aminomethyl oxodihydropyrimidinecarboxylates which underwent cyclization and resin cleavage by microwave irradiation at 150-250° for 10 min. to give II [R = Ph, 4-MeC6H4, 2-ClC6H4, 3-O2NC6H4, 4-FC6H4, 3,4-F2C6H3, 2-naphthyl, 4-BrC6H4, 3,4-(MeO)2C6H3, 2-thienyl; R1 = EtCH2, Me2CHCH2CH2, HOCH2CH2, H2C:CHCH2, c-C6H11, Ph, PhCH2, 3-MeC6H4CH2, 2-ClC6H4, 2-MeOC6H4CH2CH2, 4-FC6H4CH2CH2] in 15-55% yields. Addition of hydrazines to the resin-bound chloromethyl oxodihydropyrimidinecarboxylate intermediates at either ambient temperature gave hydrazinomethyl oxodihydropyrimidinecarboxylates which underwent cyclization and resin cleavage by microwave irradiation at 150° for 10 min. to give III [R = Ph, 2-ClC6H4, 3,4-F2C6H3, 4-BrC6H4, 3,4-(MeO)2C6H3,

2-thienyl; R2 = H, Me] in 30-41% yields. Resin cleavage in the solid-phase syntheses was traceless and did not involve addnl. steps in the preparation of the target compds.

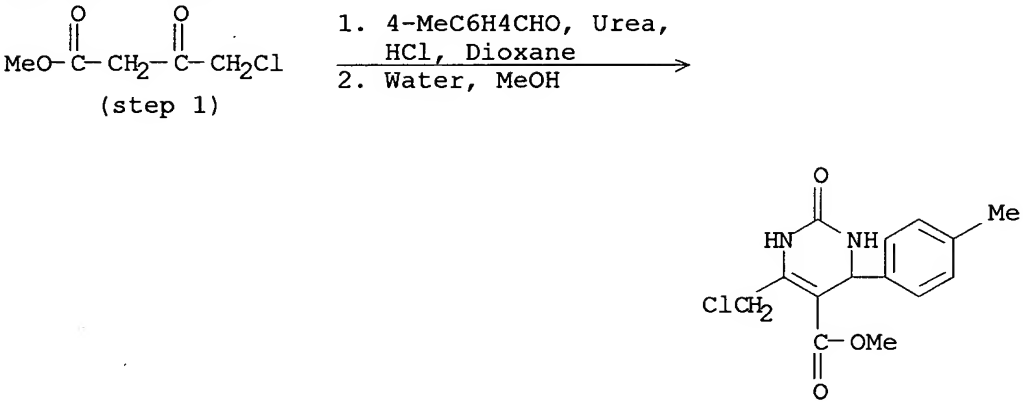
RX(9) OF 108



60%

REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: KEY STEP, Biginelli condensation

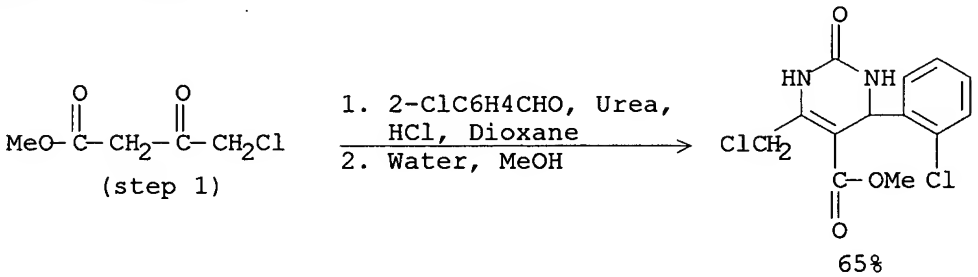
RX(10) OF 108



72%

REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: KEY STEP, Biginelli condensation

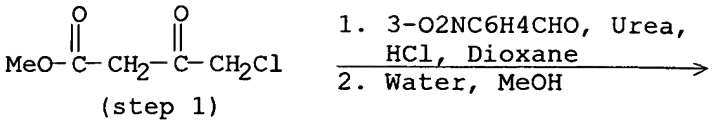
RX(11) OF 108



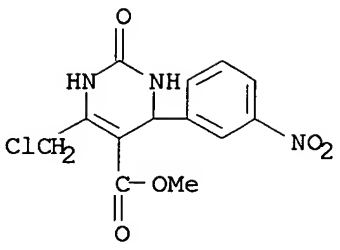
65%

REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: KEY STEP, Biginelli condensation

RX(12) OF 108



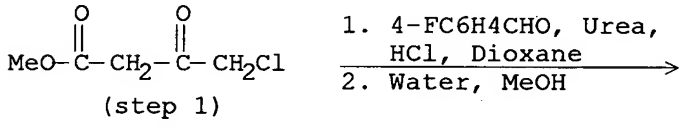
(step 1)



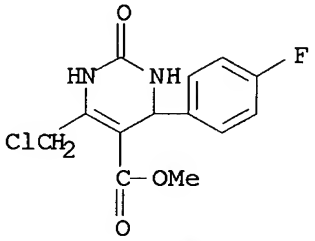
27%

REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: KEY STEP, Biginelli condensation

RX(13) OF 108



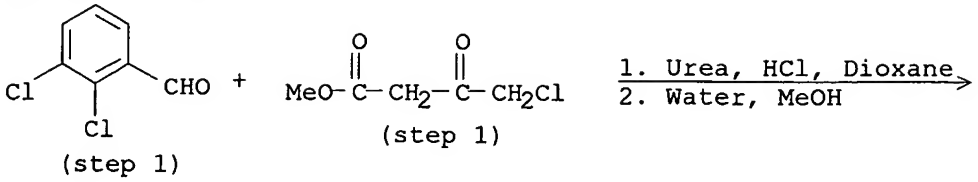
(step 1)

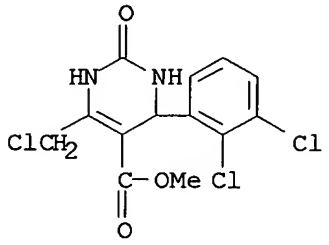


68%

REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: KEY STEP, Biginelli condensation

RX(14) OF 108

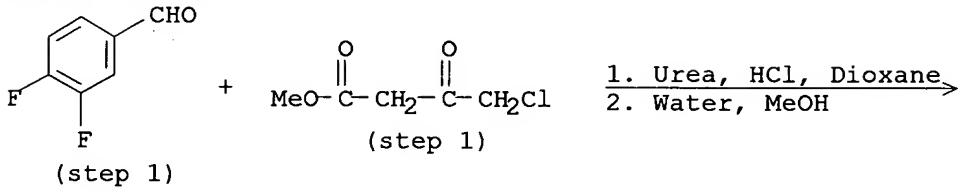


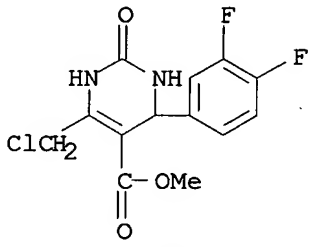


32%

REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: KEY STEP, Biginelli condensation

RX(15) OF 108

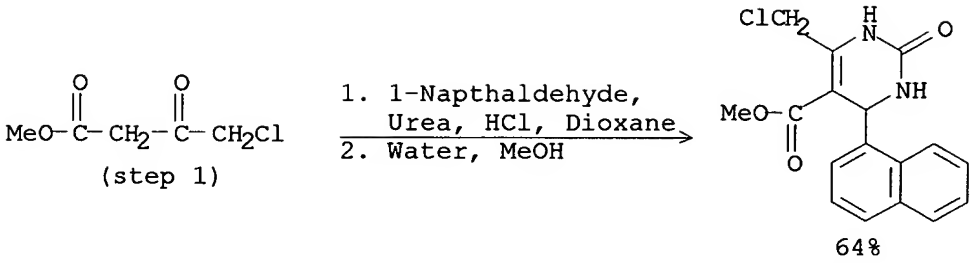




70%

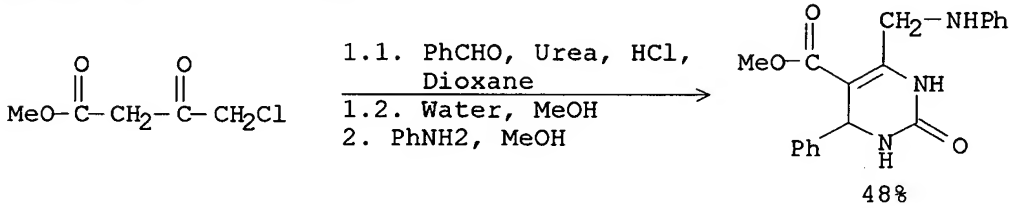
REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: KEY STEP, Biginelli condensation

RX(16) OF 108



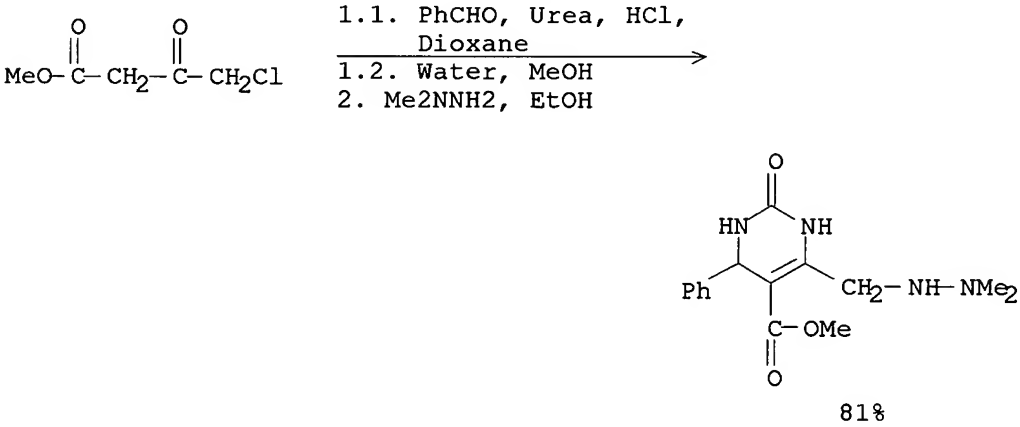
REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: KEY STEP, Biginelli condensation

RX(84) OF 108 - 2 STEPS



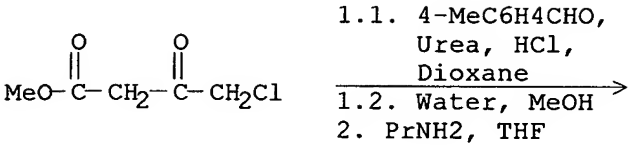
REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: 1) KEY STEP, Biginelli condensation

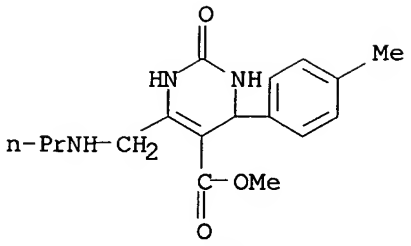
RX(86) OF 108 - 2 STEPS



REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: 1) KEY STEP, Biginelli condensation

RX(91) OF 108 - 2 STEPS





56%

REF: Journal of Combinatorial Chemistry, 4(5), 501-510; 2002
NOTE: 1) KEY STEP, Biginelli condensation

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> => log y
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               0.30     146.29

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                 ENTRY    SESSION
CA SUBSCRIBER PRICE                               0.00      -3.55

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